WHAT IS CLAIMED IS:

1. A system for the automated analysis of a set of nuclear magnetic resonance (NMR) spectral recordings of a polypeptide comprising:

(a) a library of cross-signal pattern search masks comprising masks for the specific detection of signals recorded from a fragment of the polypeptide;

(b) a selection module adapted to selecting a mask corresponding to the primary sequence of each fragment of the polypeptide;

(c) a pattern recognition module adapted to combine the various results of the cross-signal pattern search masks selected and correlate the masks to the set of NMR spectral recordings; and

(d) an assignment module adapted to assign the signals to various spin systems corresponding to the primary sequence of the polypeptide.

2. The system of claim 1, wherein the fragment comprises two or three contiguous amino acids.

3. The system of claim 1, wherein the set of NMR spectra comprises NMR experiments for the analysis of main chain signals and NMR experiments for the analysis of side chain signals.

4. The system of claim 3, wherein the NMR experiments for the analysis of the main chain signals comprise 3D experiments.

5. The system of claim 4, wherein the 3D experiments comprise CBCA (CO) NNH, CBCANNH, HA (CO) NNH, HANNH, HAHB (CO) NNH, HAHBNNH, HN (CA) CO, HNCO, HN (CO) CA and HNCA type experiments.

6. The system of claim 3, wherein the NMR experiments for the analysis of the side chain signals comprise HCCH-COSY, HCCH-TOCSY or HCC (CO) NH-TOCSY type experiments.

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7. The system of claim 3, wherein the NMR experiments for the analysis of the main chain signals and side chain signals comprise amino acid type-specific 2D experiments that are selective for an amino acid type or for a group of amino acid types.

8. The system of claim 7, wherein the amino acid type-specific 2D experiments required for the analysis of the main chain signals and side chain signals are specified corresponding to the primary sequence of the polypeptide chain.

9. The system of claim 3, wherein the NMR experiments for the analysis of the main chain signals and side chain signals comprise a combination of 2D and 3D experiments.

10. The system of claim 1, further comprising an evaluation of the NMR spectra is carried out in order to determine chemical shifts and coupling constants.

11. The system of claim 10, wherein the evaluation is carried out starting from the assignment of the NMR signals to the various spin systems of the polypeptide chain.

12. The system of claim 10, wherein the chemical shifts are collated and checked for accuracy.

13. The system of claim 12, wherein the shifts are collated and checked starting from the assignment of the NMR signals to the various spin systems of the polypeptide chain.

14. The system of claim 1, wherein the set of NMR spectra comprise spectra of the NOESY type provides information on the distances of the various nuclei of the polypeptide chain.

15. The system of claim 14, wherein the NOESY type evaluation provides information on the distances of the various nuclei of the polypeptide chain.

16. The system of claim 14, wherein the assignment of the NOESY type NMR spectra to the various nuclei of the polypeptide chain is carried out on the basis of the chemical shifts determined for the nuclei.

17. The system of claim 10, wherein results obtained from the evaluation of the NMR spectra serve as input quantities for structure calculation programs.

18. The system of claim 1, wherein the cross-signal pattern search masks comprise predefined signal search regions, wherein the NMR signals within the region boundaries provides an increased probability that the signal pattern defined by the cross-signal pattern search mask is present.

19. The system of claim 1, wherein the cross-signal pattern search masks comprise a number of predefined empty regions, wherein the absence of NMR signals within the region boundaries provides an increased probability that the signal pattern defined by the cross-signal pattern search mask is present.

20. The system of claim 1, wherein the cross-signal pattern search masks comprise threshold values and search regions determined by iteration, starting from the expected number of NMR signals in the spectra.

21. The system of claim 1, wherein the cross-signal pattern search mask comprises a plurality of sub-search masks for the analysis of the various NMR spectra of the recorded set of NMR spectra.

22. A process for the automated analysis of a set of NMR spectra, recorded for a polypeptide chain, comprising:

a) selecting a cross-signal pattern search mask from a library of cross-signal pattern search masks, wherein the mask detects a NMR signal of a fragment

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of the polypeptide chain, and wherein the selection of the required cross-signal pattern search masks is made corresponding to the fragments contained in the primary sequence;

b) executing a pattern recognition by correlating the various selected cross-signal pattern search masks with the set of NMR spectra; and

c) assigning the NMR signal to the various spin systems of the polypeptide chain corresponding to the result of the pattern recognition carried out in step b).

23. The process of claim 22, wherein the fragment of the polypeptide chain comprises two or three contiguous amino acids.

24. The process of claim 22, wherein the set of NMR spectra comprises NMR experiments for the analysis of the main chain signals and NMR experiments for the analysis of the side chain signals.

25. The process of claim 14, wherein the NMR experiments used for the analysis of the main chain signals comprises 3D experiments.

26. The process of claim 25, wherein the 3D experiments of the types CBCA (CO) NNH, CBCANNH, HA (CO) NNH, HANNH, HAHB (CO) NNH, HAHBNNH, HN (CA) CO, HNCO, HN (CO) CA and HNCA type experiments.

27. The process of claim 24, wherein the NMR experiments used for the analysis of the side chain signals comprise experiments of the types HCCH-COSY, HCCH-TOCSY and HCC (CO) NHTOCSY.

28. The process of claim 24, wherein the NMR experiments used for the analysis of the main chain signals and side chain signals comprise amino acid type-specific 2D experiments that are selective for an amino acid type or for a group of amino acid types.

29.   The process of claim 28, wherein the amino acid type-specific 2D experiments required for the analysis of the main chain signals and side chain signals are specified corresponding to the primary sequence of the polypeptide chain.

5   30.   The process of claim 22, wherein a combination of 2D and 3D experiments is used for the analysis of the main chain signals and side chain signals.

31.   The process of claim 22, further comprising evaluating the NMR spectra to determine chemical shifts and coupling constants.

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32.   The process of claim 31, wherein the evaluation is carried out starting from the assignment of the NMR signals to the various spin systems of the polypeptide chain.

15   33.   The process of claim 31, wherein chemical shifts are collated.

34.   The process of claim 33, wherein the shifts are collated starting from the assignment of the NMR signals to the various spin systems of the polypeptide chain and are checked for their correctness.

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35.   The process of claim 22, wherein the set of NMR spectra comprises spectra of the NOESY type.

36.   The process of claim 35, wherein the assignment of the NMR spectra of the
25   NOESY type to the various nuclei of the polypeptide chain is carried out starting from the chemical shifts determined for the various nuclei.

37.   The process of claim 31, wherein the quantities obtained in the evaluation of the NMR spectra are used as input quantities for structure calculation programs.

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38.   Analysis system for the automated analysis of a set of NMR spectra that has been recorded for a polypeptide chain comprising n amino acids, with a library of cross-

signal pattern search masks, in which a cross-signal pattern search mask is provided for the specific detection of the NMR signals of a fragment of the investigated polypeptide chain, with means for selecting the cross-signal pattern search masks required for the analysis from the library of cross-signal pattern search masks corresponding to the primary sequence of the polypeptide chain, the said means selecting the associated cross-signal pattern search mask for each fragment contained in the primary sequence, with means for the pattern recognition, which combine the various results of the cross-signal pattern search masks selected corresponding to the primary sequence of the polypeptide chain and correlate them to the set of NMR spectra, and with means for assigning the NMR signals to the various spin systems of the polypeptide chain corresponding to the result of the pattern recognition; wherein n is an integer greater than or equal to 2.